Anomalous transport properties of $SrTiO_3$ (STO) accumulation layers

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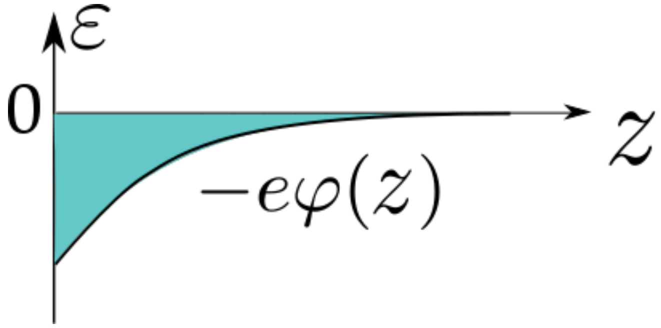
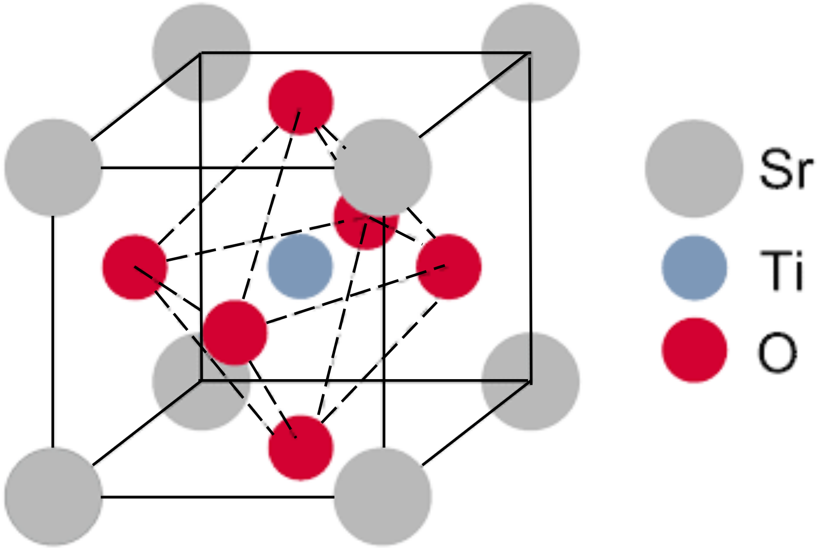
Outline

- STO accumulation layer

- Run-away tail (RAT) of electron:
  conductivity, Hall factor, thermopower



$SrTiO_3$(STO)

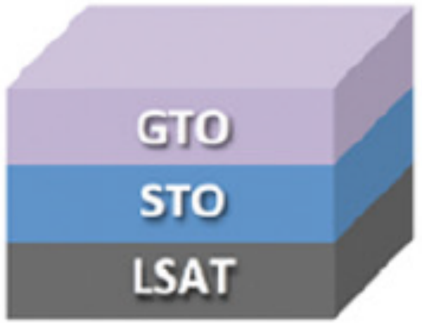


- Band insulator of gap 3.2 eV
- Quantum paraelectric, κ=20000
- Lattice constant a=3.9 Å

Motivation

- Heterostructures: $LaAlO_3$(LAO)/STO, $GdTiO_3$(GTO)/STO, GTO/STO/GTO, etc.

[P. Moetakef, *et al.*, Applied Physics Letters 99, 232116 (2011)]



- Superconductivity, magnetism, multiferroics
- Electronic structure and transport

Accumulation layer

- $N = 10^{13} \sim 10^{14}\ \mathrm{cm}^{-2}$

- Local degenerate gas: Thomas Fermi (TF) approximation

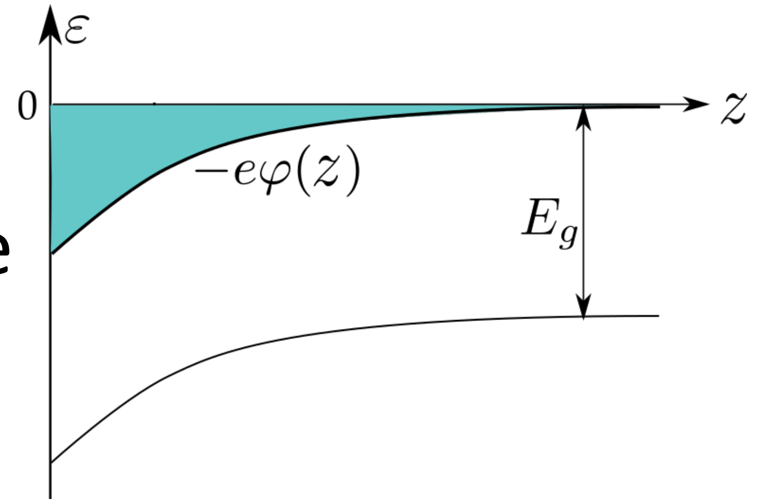
$$n(r) = \mathrm{Const.}/b^3\ [\varphi(r)/e/b]^{3/2},\quad b = \hbar^2/m^* e^2$$

- Self-consistent screening

$$\nabla \cdot D = -4\pi e n(r)$$

- Nonlinear dielectric response

$$\vec{D} \neq -\kappa \nabla \varphi$$



Nonlinear dielectric response

$E \approx 4\pi P/\kappa + P^3/P_0^2$ $P_0 \approx e/a^2 \gg P$

$\ll P$

$D = E + 4\pi P \approx 4\pi P$

$-\nabla\varphi = E \propto D^3$

$\nabla D = -4\pi e n(r)$

$\frac{d}{dz}\left[\left(\frac{d}{dz}\frac{\varphi}{e/a}\right)^{1/3}\right] = \frac{\text{Const.}}{a^{4/3}}\left(\frac{\varphi}{e/a}\right)^{3/2}$

Electron distribution

- Potential and density profile

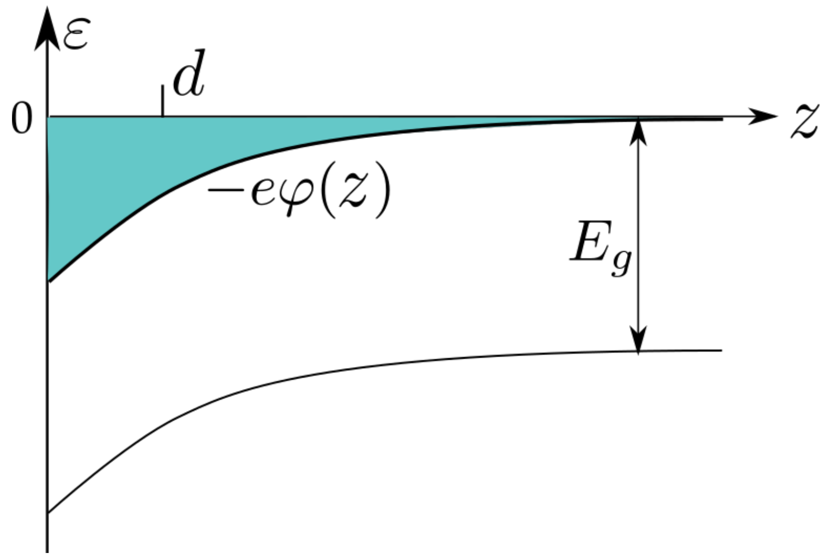
$$\varphi(z) \approx \frac{e}{a}\left(\frac{a}{z+d}\right)^{8/7}, \qquad n(z) \approx \frac{1}{a^3}\left(\frac{a}{z+d}\right)^{12/7}$$

- Characteristic decay length

$$d \approx a\left(Na^2\right)^{-7/5} > a,$$

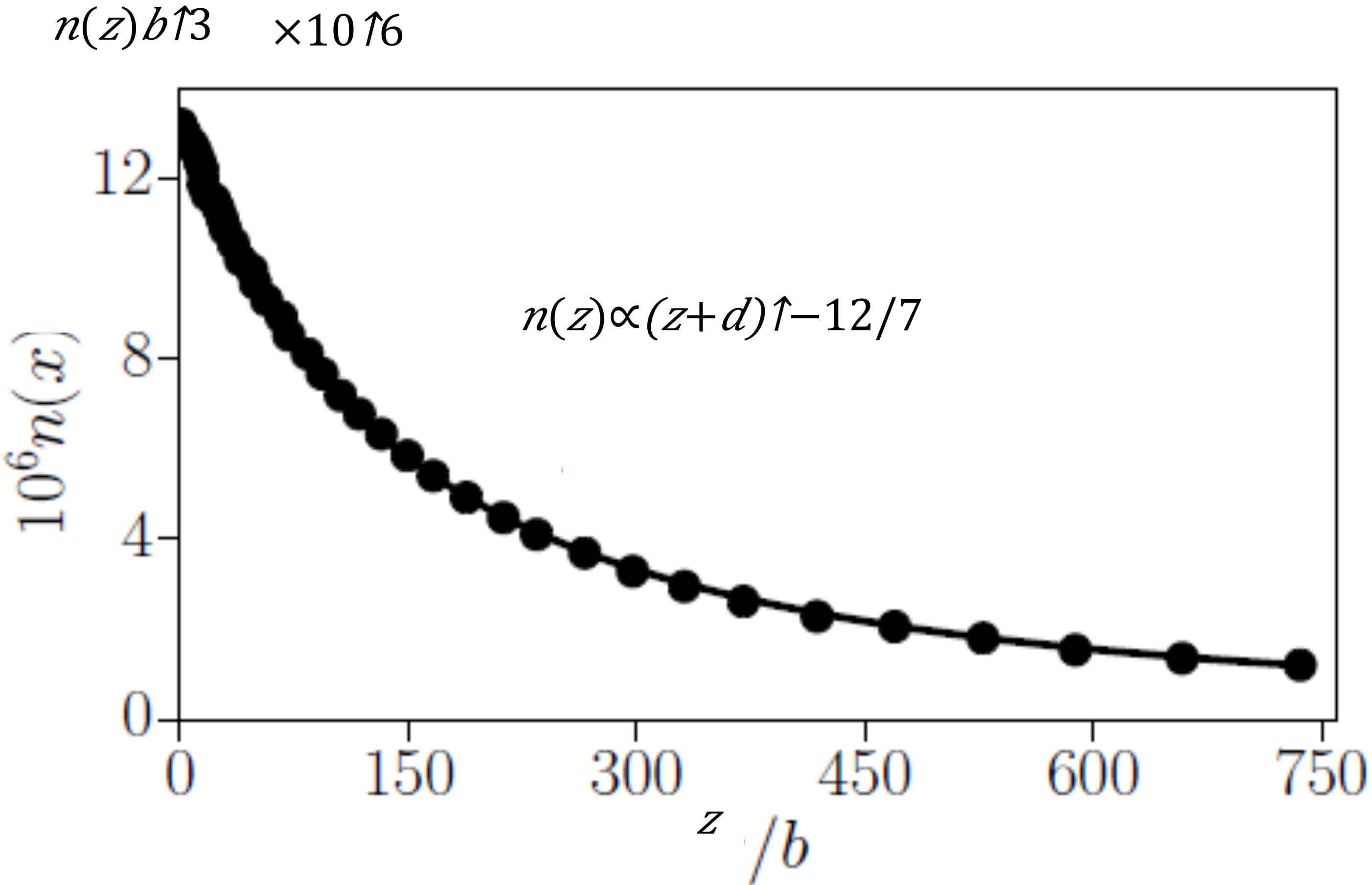
$$Na^2 < 1$$

[K. V. Reich *et al*, PRB 91, 115303 (2015)]



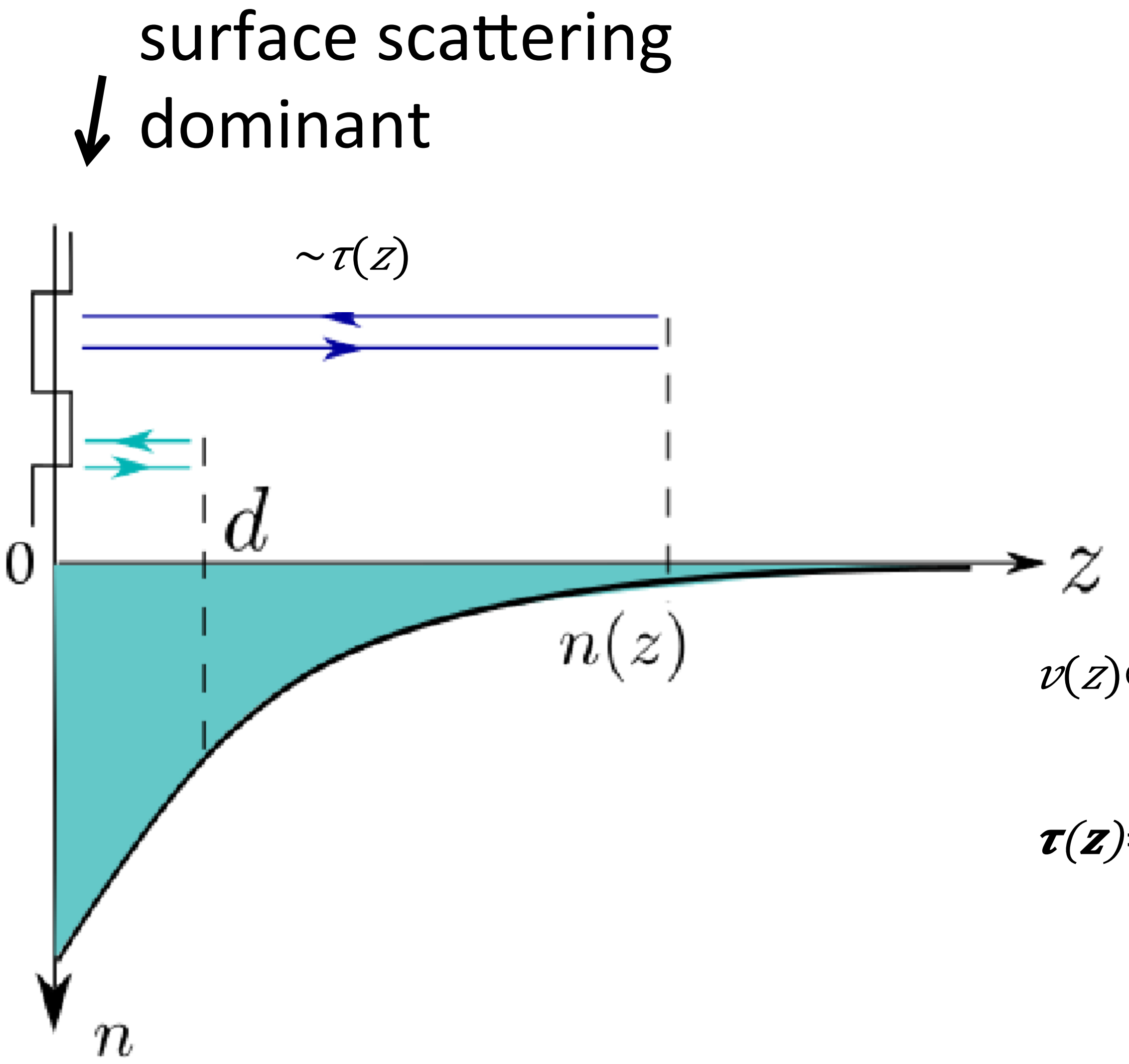
Comparison with experiments

- LAO/STO by Hwang *et al*, 2014



[K. V. Reich *et al*, PRB 91, 115303 (2015)]

Run-away tail (RAT)



$\tau(z) \sim z/v(z)$

$n(z) \propto z^{-12/7}$

$v(z) \propto [n(z)]^{1/3} \propto z^{-4/7}$

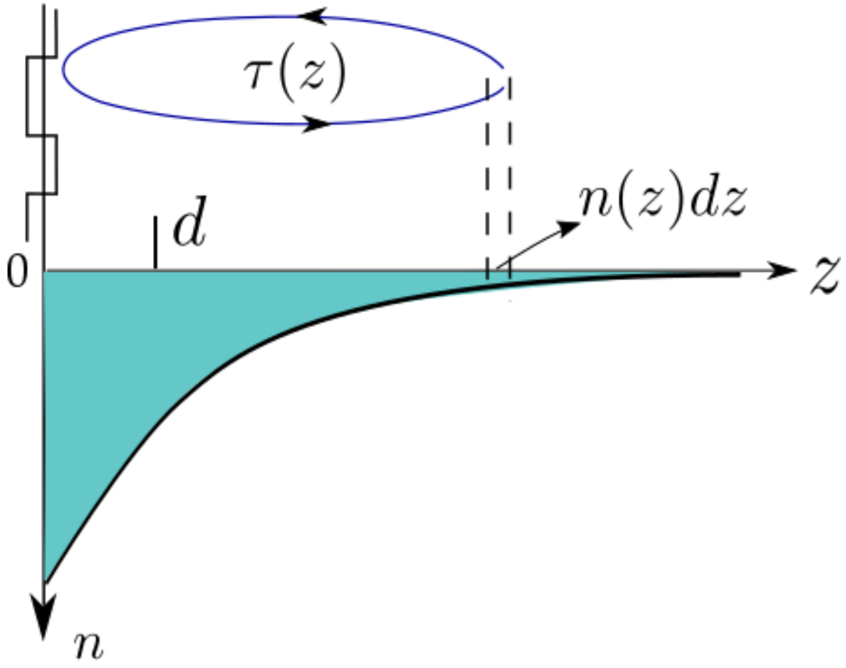
$\boldsymbol{\tau(z) = \tau_s (z/d)^{11/7}}$

Divergent conductivity

- $\sigma = Ne^2 \langle\tau\rangle / m^*$

$$\langle\tau\rangle = N^{-1} \int_0^L dz\, n(z)$$

$$\propto \int_0^L z^{-1/7}$$



- $\langle\tau\rangle = \tau_s (L/d)^{6/7} \gg \tau_s$

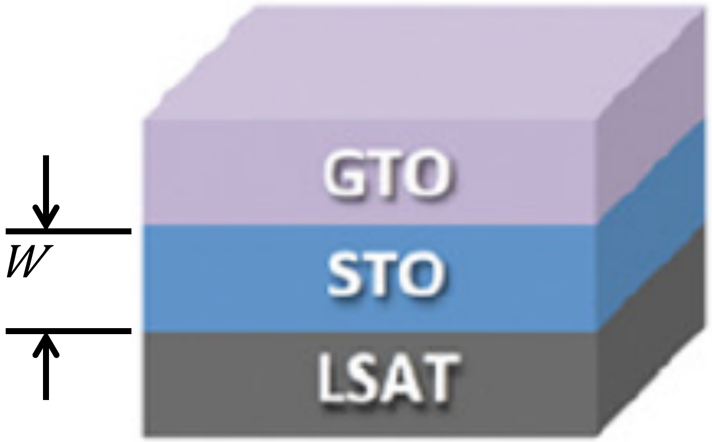
divergent conductivity

- $\sigma = \sigma_s (L/d)^{6/7} \gg \sigma_s$, $\sigma_s = N e^2 \tau_s / m^*$

Truncation length L

- Finite sample width W (thin quantum wells)

$$\sigma=\sigma_s (W/d)^{6/7}$$



[P. Moetakef, *et al.*,
Applied Physics Letters
99, 232116 (2011)]

Hall factor

- Hall coefficient

$$R_H = r_H / Nec$$

- Hall factor at small magnetic fields

$$r_H = \langle \tau^2 \rangle / \langle \tau \rangle^2 , \quad \langle \dots \rangle = N^{-1} \int_0^L dz\, n(z) \dots$$

- Two-band model at low magnetic fields

$$R_H = 1/ec \, (N_1 \mu_1^2 + N_2 \mu_2^2)/(N_1 \mu_1 + N_2 \mu_2)^2 , \; N = N_1 + N_2$$

Anomalous Hall factor

- $r_H = \langle \tau^2 \rangle / \langle \tau \rangle^2$, $\tau(z) \propto z^{11/7}$, $n(z) \propto z^{-12/7}$

$$\langle \tau^2 \rangle = \tau_s{}^2 (L/d)^{17/7}, \quad \langle \tau \rangle = \tau_s (L/d)^{6/7}$$

$$r_H = (L/d)^{5/7} \gg 1,$$

- Finite sample width W

$$r_H = (W/d)^{5/7} \gg 1$$

Truncation by magnetic field

- Truncation by magnetic field (nonlinear Hall effect)

$\omega_c \tau(L)=1,$ $\omega_c = eB/m^*$

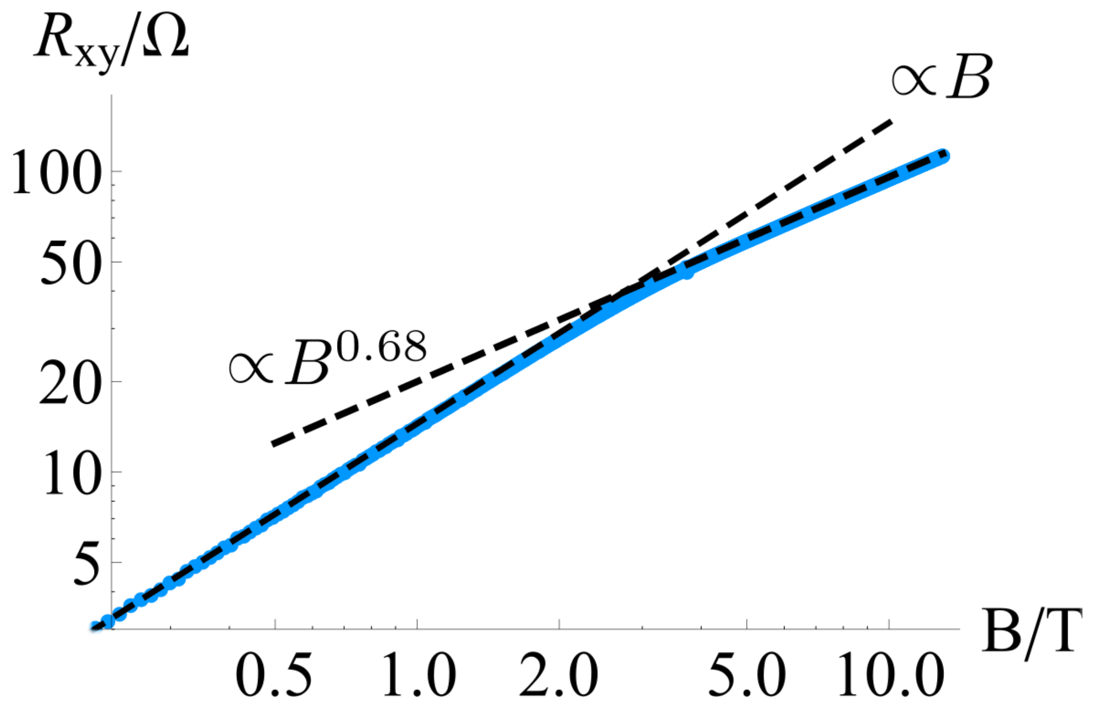
$$r_H \propto B^{-5/11}$$

$$R_{xy} = B/ec\, r_H/N \propto B^{6/11}$$

nonlinear Hall effect

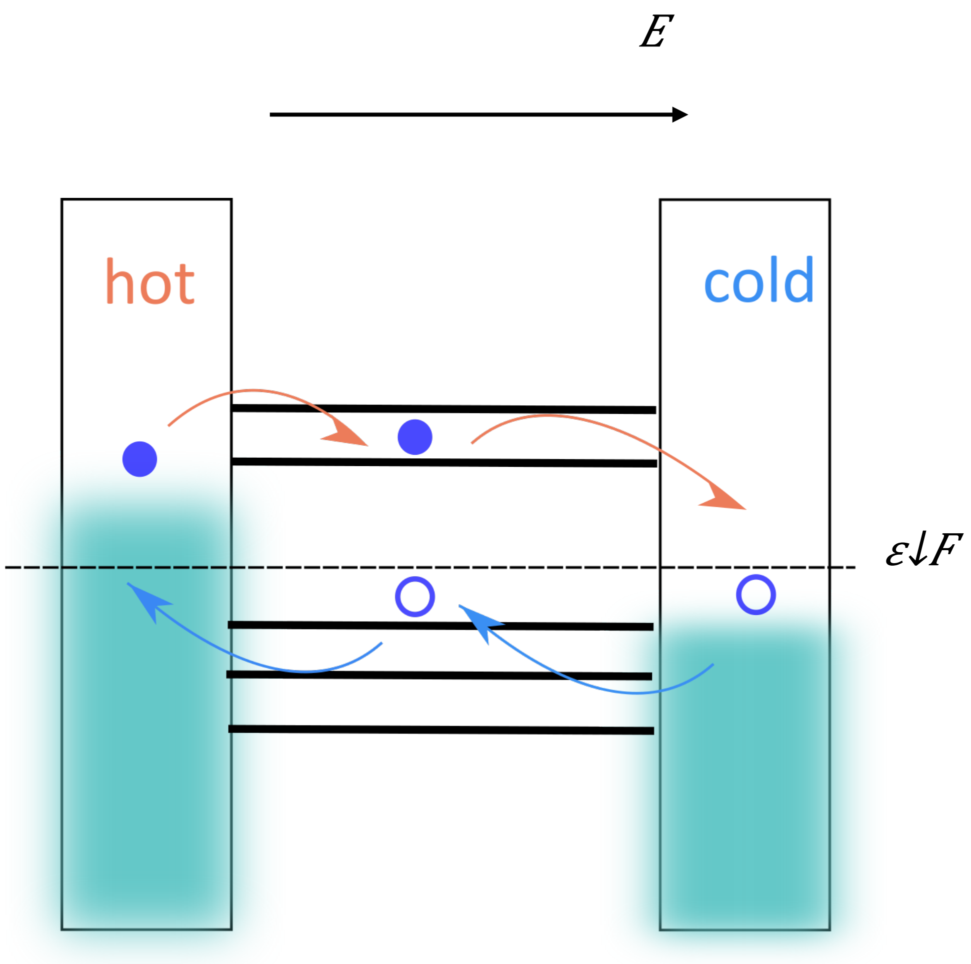
Comparison with experiments

- Theoretical prediction: $R_{xy} \propto B^{\alpha}$, $\alpha \approx 0.55$
- Experimental fitting: at largest N, $\alpha \approx 0.68 \pm 0.04$



Original data are from Hwang's group for their work Nano Lett., 2016, 16 (10), pp 6130

Thermopower S



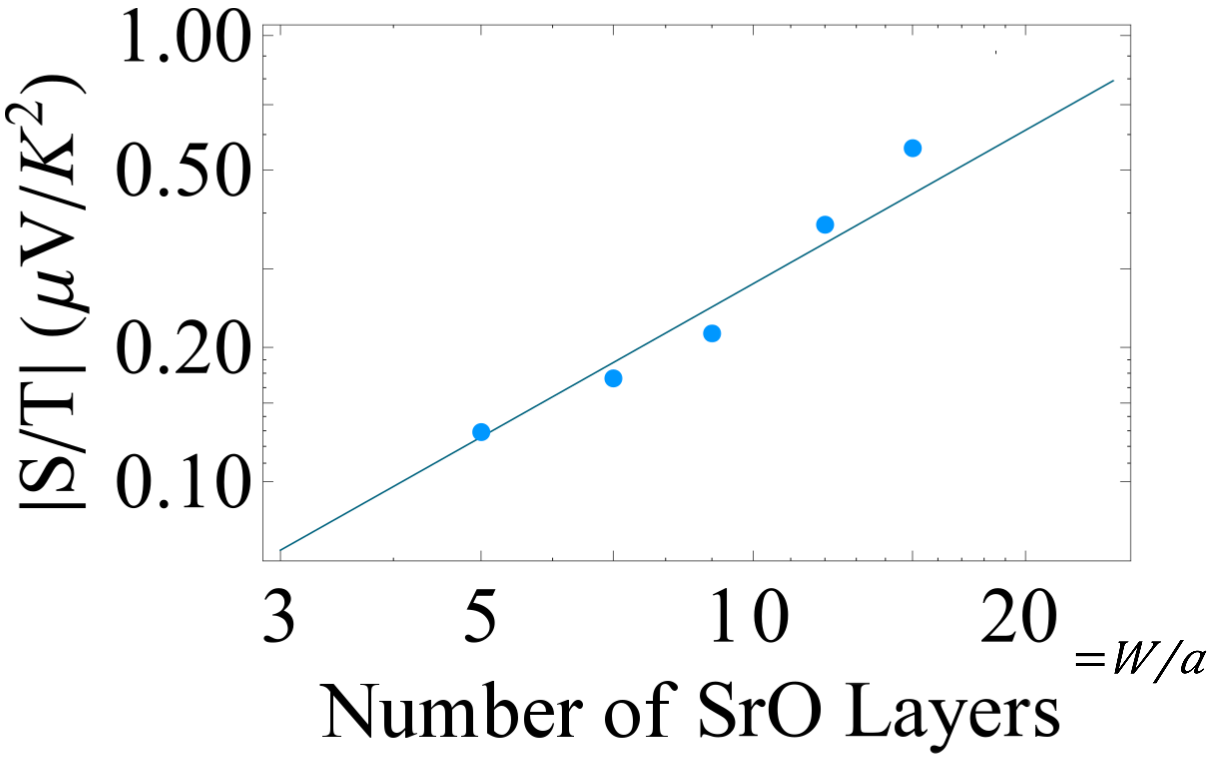
- $S = |E/\nabla T| \simeq k_B^2 T/e \, \langle \tau/\varepsilon \rangle / \langle \tau \rangle \propto \langle \tau/n^{2/3} \rangle / \langle \tau \rangle$

- For thin samples

$$S/T \propto (\boldsymbol{W/d})^{\mathbf{8/7}}$$

Comparison with experiments

- $S \propto W^{8/7}$ agrees reasonably well with the extracted experimental data



GTO/STO/GTO

GTO: $GdTiO_3$

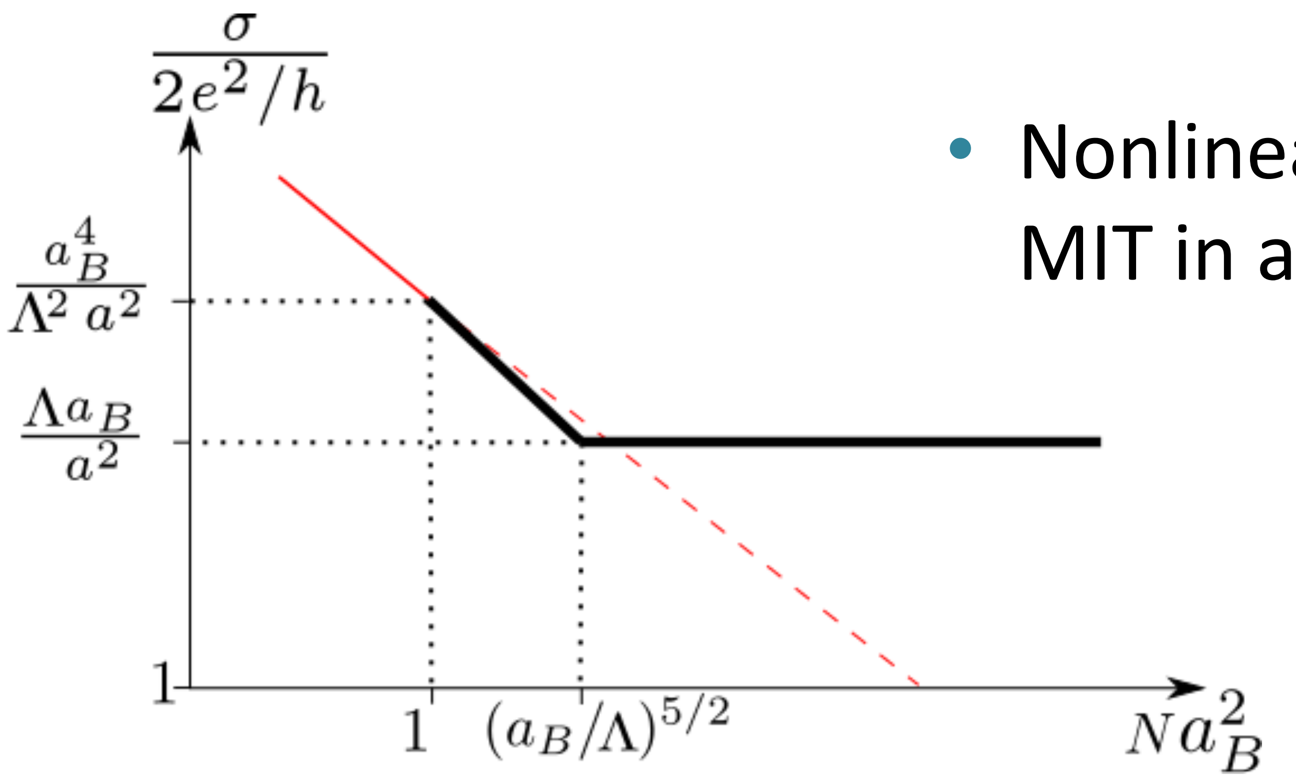
[T. A. Cain, *et al.*, arXiv:1609.04149]

Summary

- $n(z) \propto z^{-12/7}$ tail in STO accumulation layers due to nonlinear dielectric response
- $\tau(z) \propto z^{11/7}$ run-away tail (RAT) by surface scattering yielding the divergent kinetic coefficients
- Consistency with the experimental nonlinear Hall effect and scaling behavior of the thermopower

Surface roughness scattering of multi-subband accumulation layer

- Linear dielectric response: no reentrant metal-insulator transition (MIT) conjectured by Das Sarma, *et al.*, in 2014



- Nonlinear: no reentrant MIT in available N range

Truncation by bulk scattering

- Bulk scattering rate $1/\tau_b$

$$\tau(L)=\tau_b$$

$$\sigma=Ne\mu$$

$$\mu=\mu_s^{5/11}\mu_b^{6/11}\gg\mu_s,$$

$$\mu_s=e\tau_s/m^*, \qquad \mu_b=e\tau_b/m^*$$

Truncation by linear crossover

- Crossover to linear dielectric response (with dielectric constant κ)

$$E \approx 4\pi P/\kappa + P^3/P_0^2$$

$$L \approx a\kappa^{7/10}$$

$$z \gg L, \quad n(z) \propto z^{-6}$$

[Frenkel 1928]

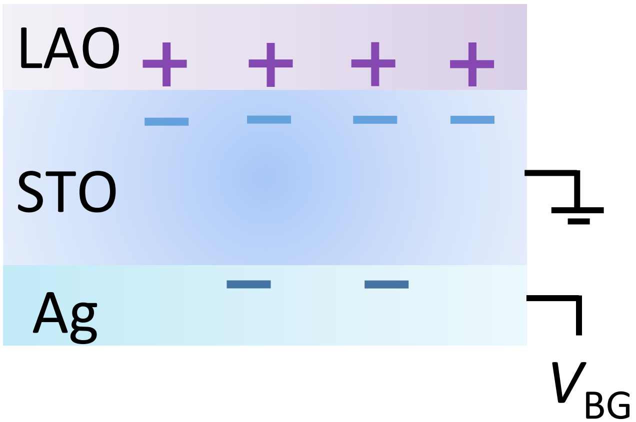
Truncation by backgate voltage

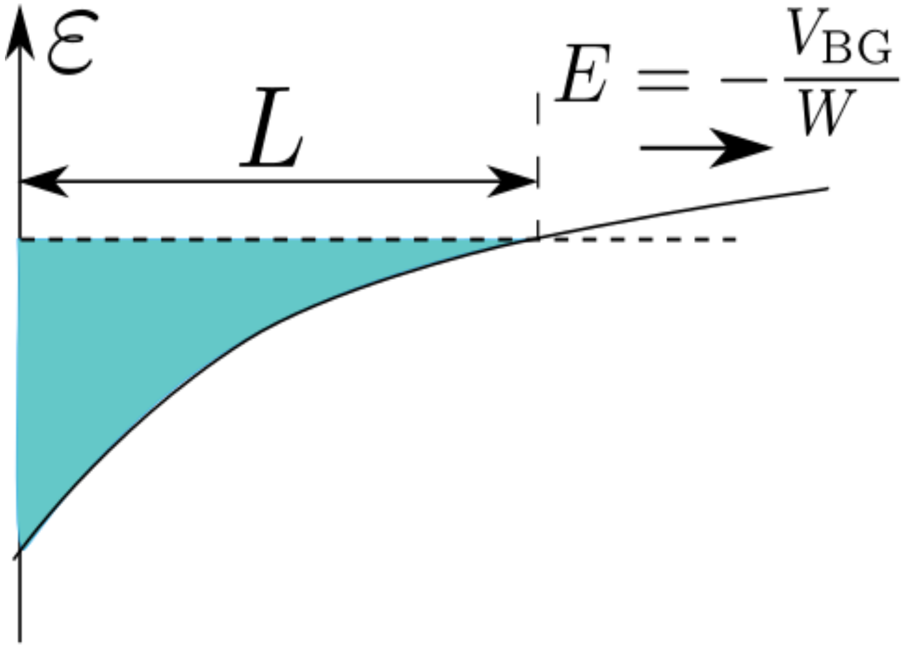
- Back gate with voltage V_{BG}

$$E(L) = -d\varphi/dz\,(L) = -V_{BG}/W$$

$$\sigma \propto |V_{BG}|^{-2/5}$$

$$r_H \propto |V_{BG}|^{-1/3}$$

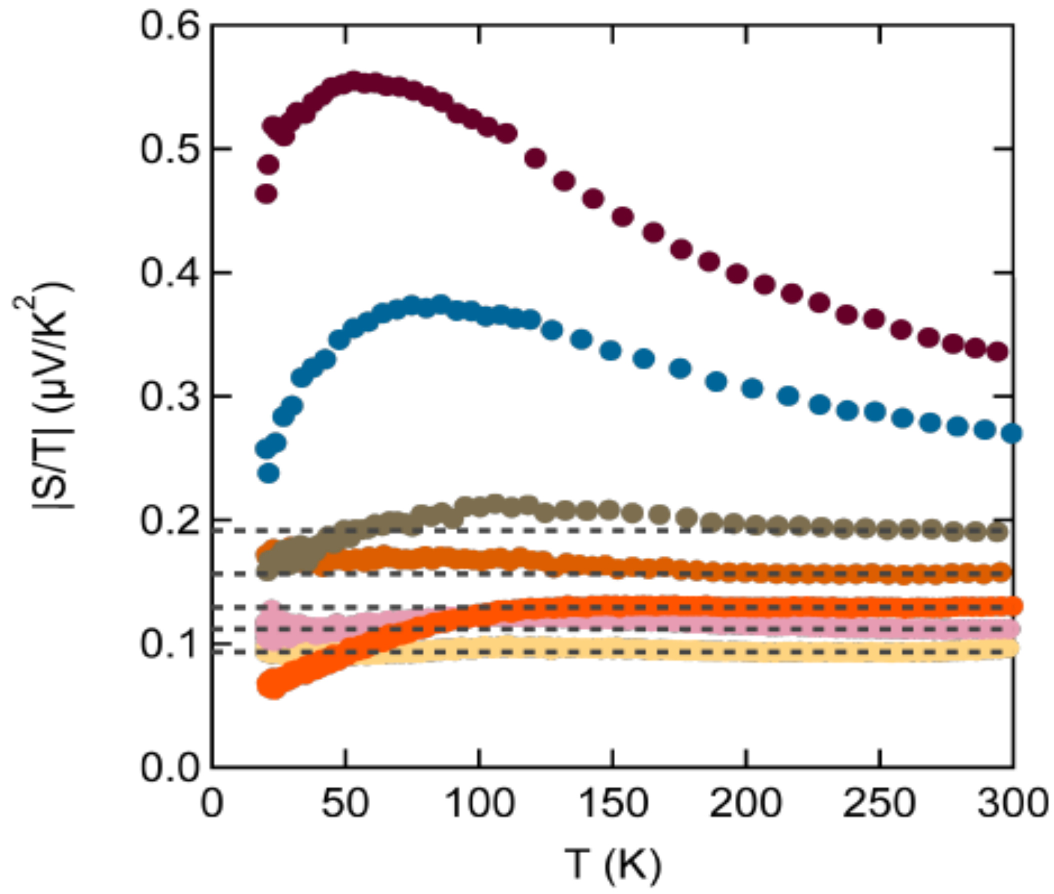




Comparison with experiments

- Thermopower S

[T. A. Cain, *et al.*, arXiv:1609.04149]

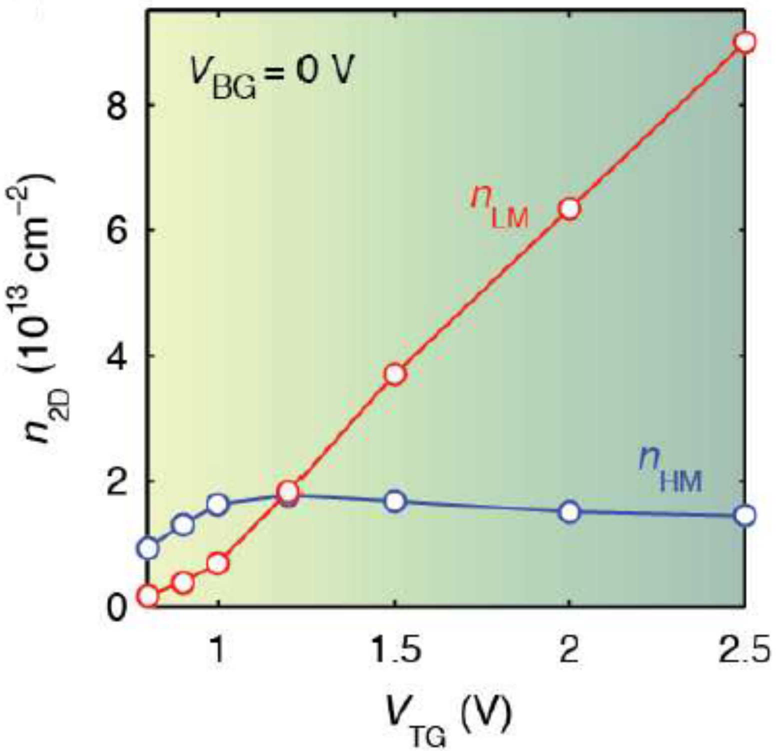


GTO/STO/GTO

GTO: $GdTiO_3$

Two-band model

V_{TG} /V	1.5	2.0	2.5
n_{LM} /10^{13} cm^{-2}	~3.8	~6.3	~9.0
n_{HM} /10^{13} cm^{-2}	~1.5	~1.5	~1.5



- $n_{LM}/n_{HM} \neq n_{d_{xy}}/n_{d_{xz+yz}}$

[Zhuoyu Chen, *et al.*, Nano Lett., 2016, 16 (10), pp 6130–6136]

Multi-band Drude model

$$\sigma_{i,xx} = \frac{\sigma_i}{1+\omega_c^2 \tau_i^2} = \frac{N_i e \mu_i}{1+\mu_i^2 B^2}, \quad \sigma_{i,xy} = \frac{N_i e \mu_i^2 B}{1+\mu_i^2 B^2}$$

$$\sigma_{xx} = \sum_i \sigma_{i,xx}, \quad \sigma_{xy} = \sum_i \sigma_{i,xy},$$

$$R_{xy} = \frac{\sigma_{xy}}{\sigma_{xx}^2 + \sigma_{xy}^2} = R_H B,$$

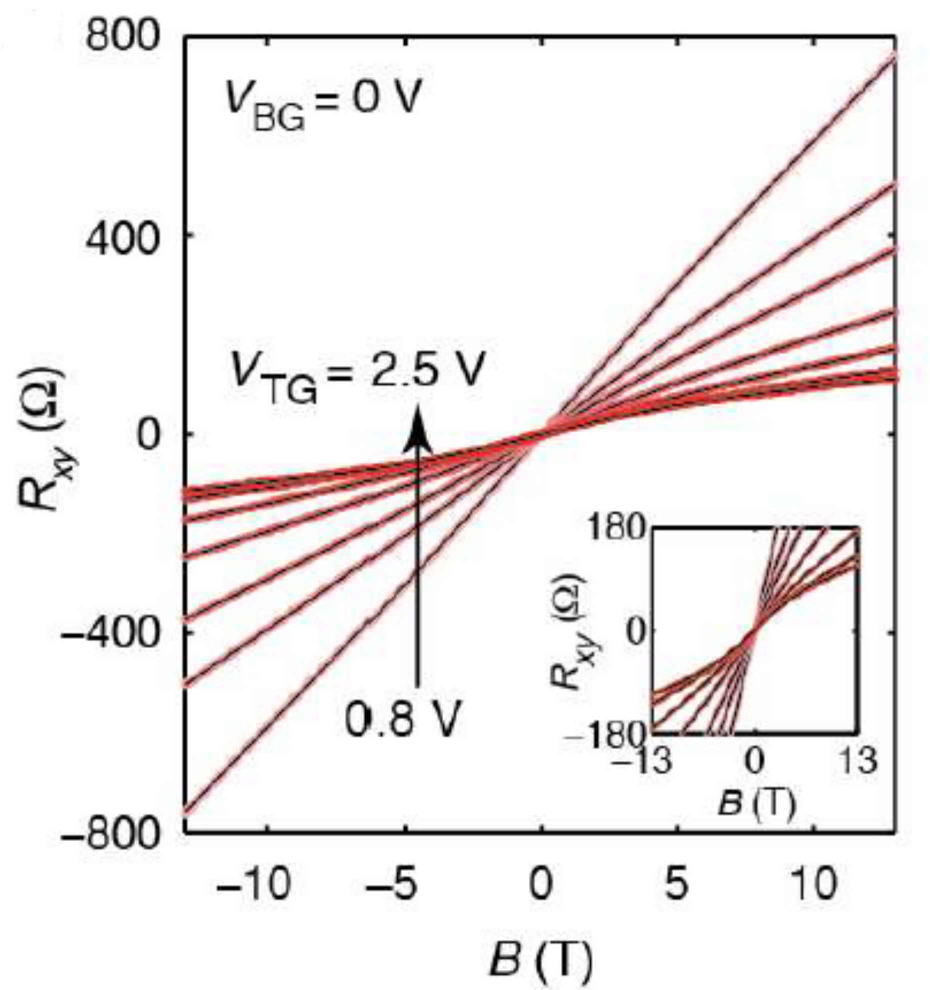
$$R_H = \frac{1}{e} \frac{\left(\sum_i \frac{N_i \mu_i^2}{1+\mu_i^2 B^2}\right)}{\left(\sum_i \frac{N_i \mu_i}{1+\mu_i^2 B^2}\right)^2 + \left(\sum_i \frac{N_i \mu_i^2 B}{1+\mu_i^2 B^2}\right)^2}$$

Comparison with experiments

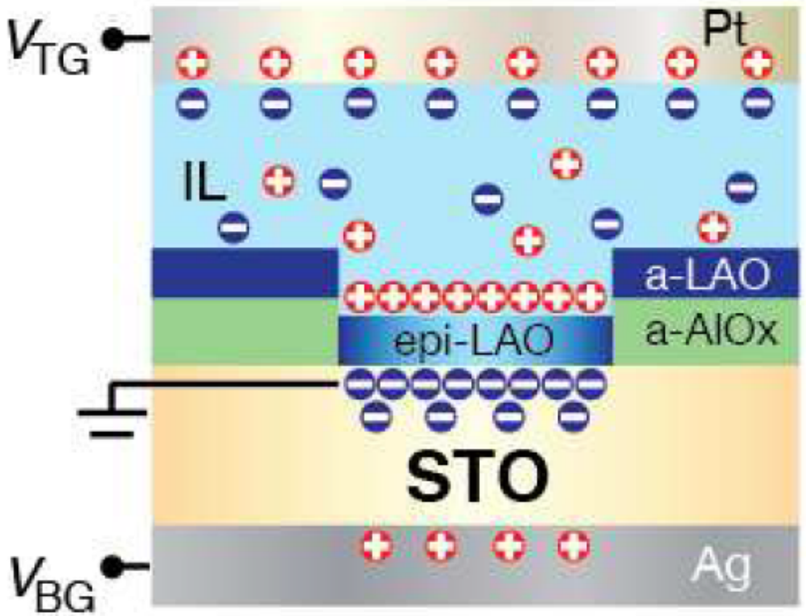
- Nonlinear Hall effect: $r_H = (L/d)^{5/7}$ at small magnetic fields,
- L is intrinsic truncation length
- $n_{0\mathrm{T}} = n_t/(L/d)^{5/7}$, $n_\infty = n_t$
- At intermediate B, truncation length is determined by $\omega_c \tau(L_B)=1$, $L_B \propto B^{-7/11}$

$$R_{xy} \propto B^{6/11}$$

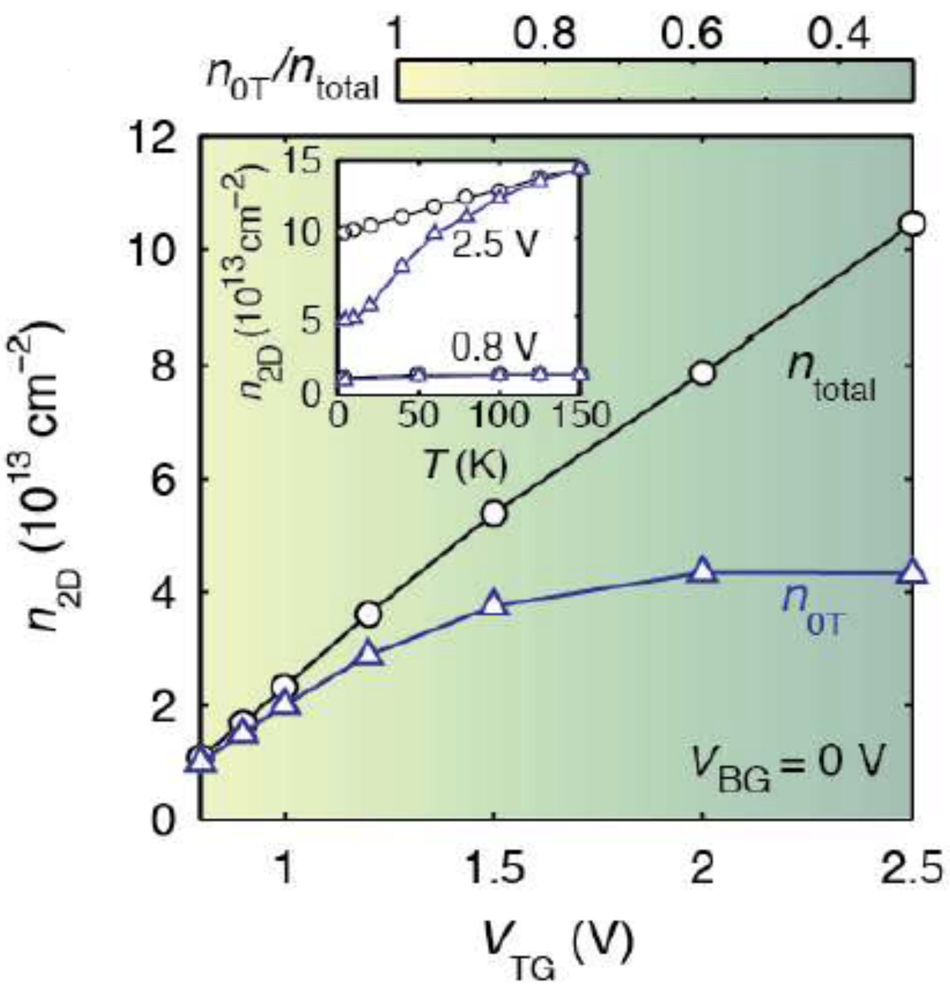
Comparison with experiments



[Zhuoyu Chen, *et al.*, Nano Lett., 2016, 16 (10), pp 6130–6136]



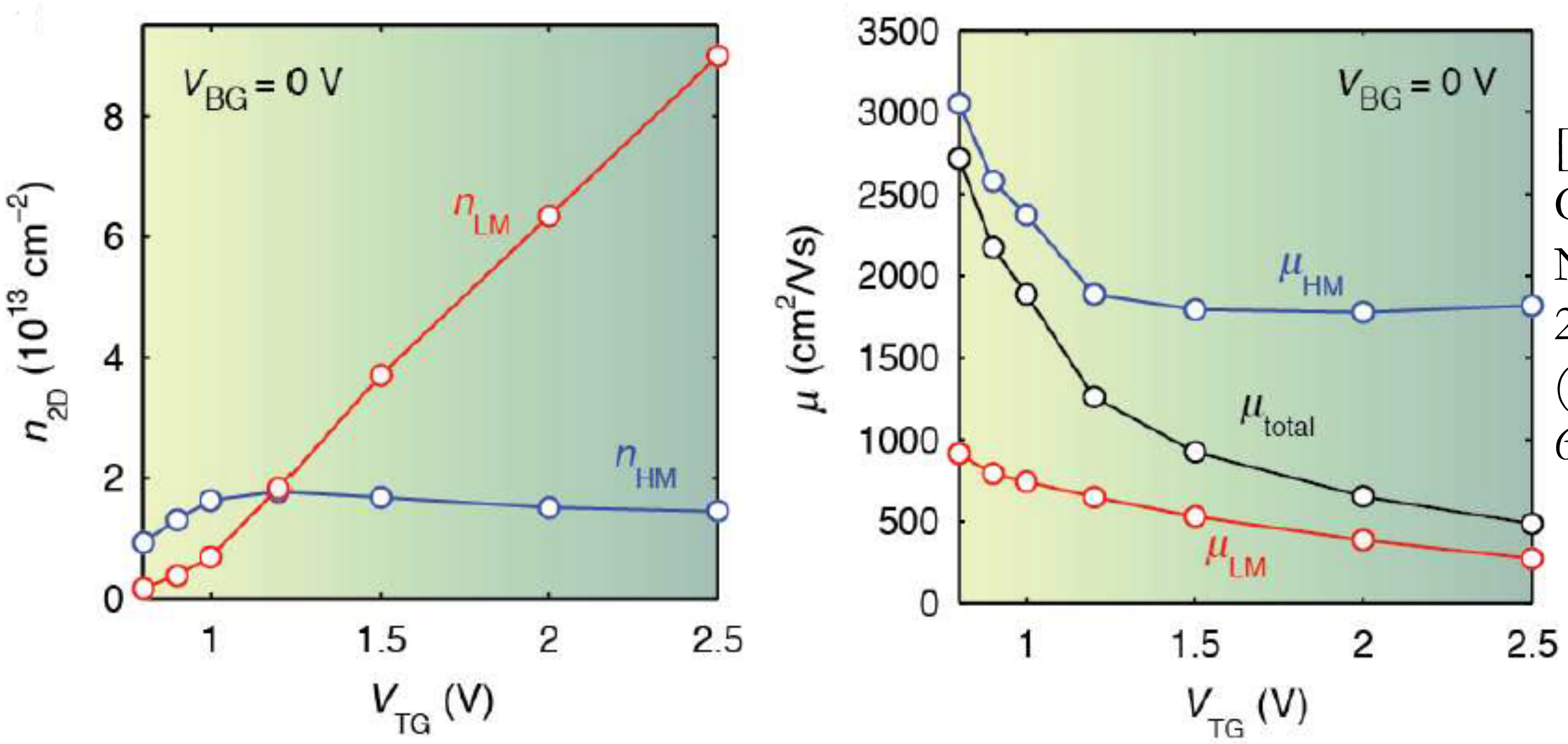
Comparison with experiments



Comparison with experiments

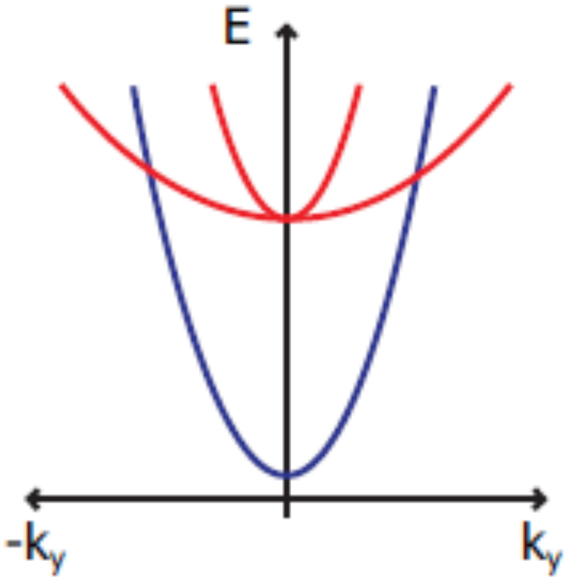
- High mobility electrons → tail electrons

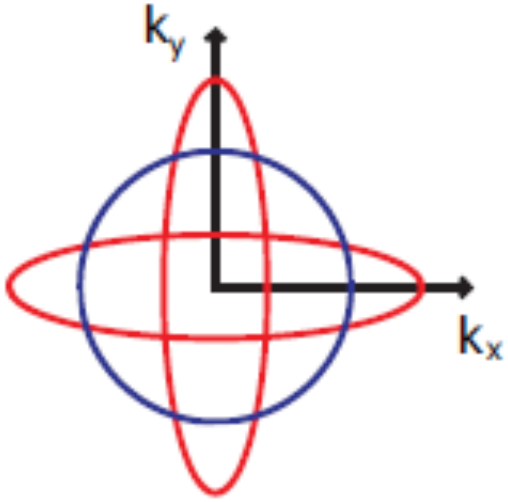
  low mobility electrons → body electrons



[Zhuoyu Chen, *et al.*, Nano Lett., 2016, 16 (10), pp 6130–6136]

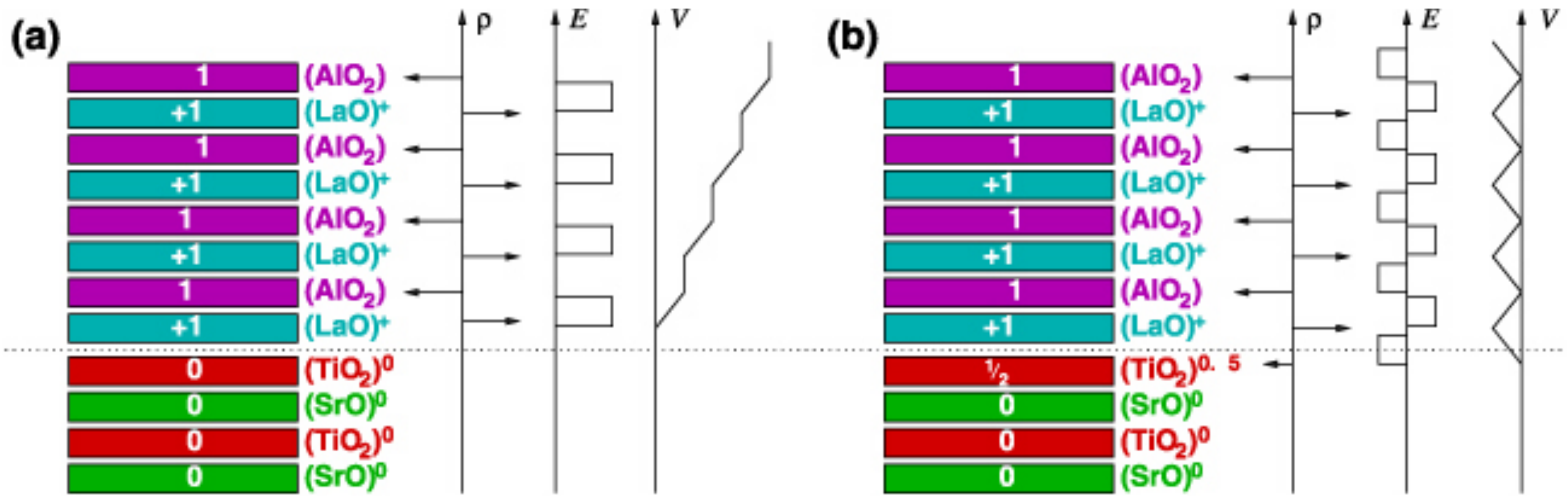
Band structure in STO





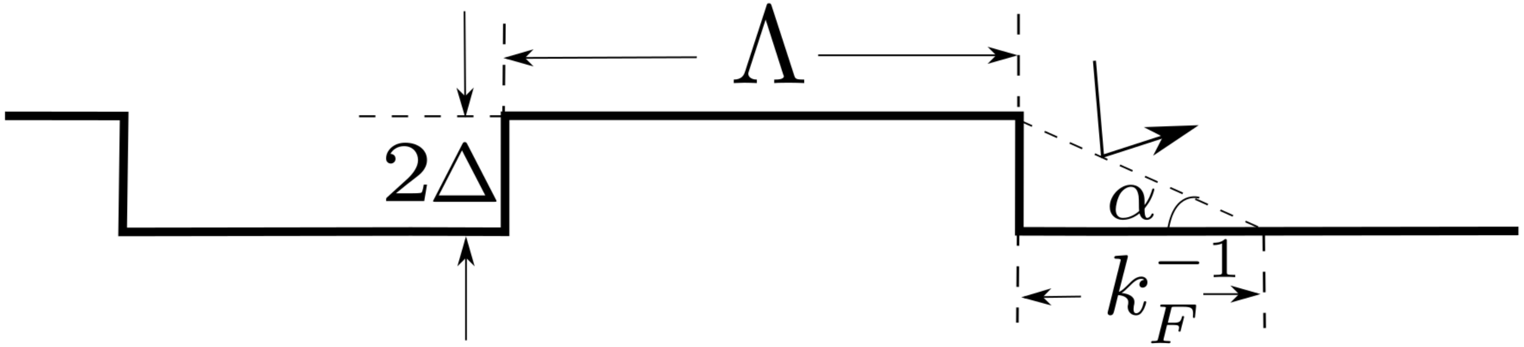
[J. R. Tolsma, *et al.*, arXiv:1608.03625]

Polar catastrophe



Surface scattering mechanism

- Surface roughness $\Lambda \gg k_F^{-1}$, $\Delta \sim a \ll \Lambda$



- Time to the surface: d/v_F
- Probability to scatter: k_F^{-1}/Λ

[Han Fu, *et al.*, Phys. Rev. B 93, 235312 (2016)]

[Han Fu, *et al.*, Phys. Rev. B 94, 045310 (2016)]

Surface roughness scattering

- Deviation angle: $\alpha \sim \Delta / k_F^{-1}$
- Scattering rate: $\alpha^2 v_F / d \, k_F^{-1} / \Lambda = \hbar / m^* \, \Delta^2 k_F^2 / d\Lambda$
- $\mu_s \sim e/\hbar \, \Lambda d / \Delta^2 k_F^2$